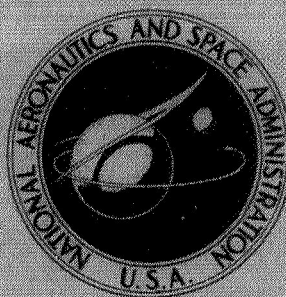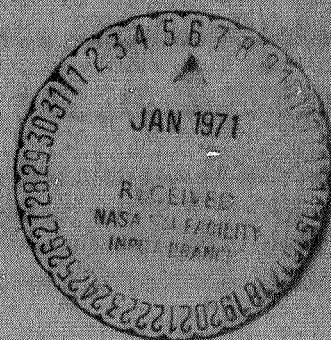**NASA TECHNICAL MEMORANDUM**

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DUAL-CHANNEL SPECTROMETER FOR ROTATIONAL-TEMPERATURE MEASUREMENTS

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and William W. Hunter, Jr.

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Hampton, Va. 23365

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16. Abstract

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TEMPERATURE MEASUREMENTS

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SUMMARY

A unique dual-channel spectrometer capable of making rotational-temperature measurements of low-density (1.5×10^{22} m^{-3}) nitrogen gas up to 550° K has been developed and tested. The instrument images on a single variable-width (0 to 500 μm) entrance slit the fluorescence of the first negative system of nitrogen resulting from inelastic collisions between fast electrons and nitrogen molecules. The rotational energy interval observed by each channel is set by preselected exit slit widths. The ratio of rotational energy within the two channels is then a calculable function of temperature. To understand quantitatively the effect of entrance slit width on the energy ratio between the two channels, a model spectrum of the N_2^+(0-0) and N_2^+(1-1) vibrational bands of nitrogen was calculated. By integration of the model spectrum over the limits set by the exit slits, it was possible to calculate a series of energy ratios for different temperatures at various entrance slit widths. The calculated effect of the entrance slit width on temperature measurements was in good quantitative agreement with the laboratory results.

INTRODUCTION

This work was undertaken in an effort to improve the technique of measuring the rotational temperature of low-density nitrogen gas. In the past this technique has involved either scanning a vibrational band of nitrogen with a spectrometer or comparing two parts of a vibrational band with a two-filter system. The first method is rather slow in that up to several minutes may be involved in a scan, in addition to the time necessary to reduce the data; the filter method, although faster, severely attenuates a significant amount of information in the vibrational band. There are also several other problems with a filter system. Because of the grouping of the more intense vibrational bands, the filters will pass some of the energy from adjacent bands; this can cause some difficulty if the vibrational temperature is unknown, although this work was done with the rotational and vibrational modes in equilibrium. It can be shown, however, that the uncertainty introduced by an unknown vibrational temperature is not great. The main problem is that

the filters have wings which cause a significant overlap when the two filters peak near one another. Since one filter observes much of the band in common with the other filter, a loss occurs in resolving changes within the band. An additional problem lies in the instability of narrow-band interference filters under changing ambient conditions.

The instrument described in this report is a dual-channel spectrometer with a single entrance slit. Instead of scanning the spectrum chosen for rotational-temperature measurements, each channel observes the intensity of one of two nonoverlapping sections of the spectrum, and from the relative distribution of rotational spectral energy, the rotational temperature can be determined. The foundation for this work was developed by E. P. Muntz (ref. 1) and the theoretical work covered in this paper is based considerably on his contributions.

With this instrument it is now possible to make high-response rotational-temperature measurements in low-density nitrogen gas. These measurements can be made with greater accuracy and speed and lower light levels than heretofore.

SYMBOLS

B_0 rotational constant related to vibrational level $V_1'' = 0$

c speed of light

h Planck's constant

$I_{K',K'+1}$ strength of rotational line emitted in decay from rotational quantum state K' to state $K' + 1$ (P branch)

$I_{K',K'-1}$ strength of rotational line emitted in decay from rotational quantum state K' to state $K' - 1$ (R branch)

I_λ intensity at any wavelength λ

$I_{\lambda\ell}$ intensity at the center of a spectral line

K_1'' rotational quantum number of neutral ground state

K' rotational quantum number of first excited ionized state of nitrogen

K_2'' rotational quantum number of ground ionized state

k	Boltzmann's constant
$N_2^+(0\text{-}0)$	the (0-0) vibrational band in the first negative system of nitrogen
$N_2^+(1\text{-}1)$	the (1-1) vibrational band in the first negative system of nitrogen
$N_2^+ X^2\Sigma_g^+$	ground ionized state of nitrogen
$N_2 X^1\Sigma_g^+$	neutral ground state of nitrogen
$N_2^+ B^2\Sigma_u^+$	first excited ionized state of nitrogen
T_r	rotational temperature
V_1''	vibrational quantum number of neutral ground state
V'	vibrational quantum number of first excited ionized state
V_2''	vibrational quantum number of ground ionized state
W_l/W_v	ratio of Lorentz line width to Voigt line width
λ	wavelength
$\lambda_{\mathbb{C}}$	wavelength of the center of a spectral line
ν	wave number

THEORETICAL BASIS FOR MEASUREMENTS

An electron beam of 28-keV electrons was used to excite the neutral $N_2 X^1\Sigma_g^+$ nitrogen molecule to the $N_2^+ B^2\Sigma_u^+$ excited ionized state, from which the molecule spontaneously decays to the ground ionized state $N_2^+ X^2\Sigma_g^+$ with the emission of a photon. (See fig. 1.) The relative population distributions of the vibrational and rotational molecular states of $N_2 X^1\Sigma_g^+$ are functions of the vibrational and rotational temperature, respectively. By use of an analysis of the spectrum produced by the $N_2^+ B^2\Sigma_u^+$ molecule, determination of the temperature in the ground state is possible.
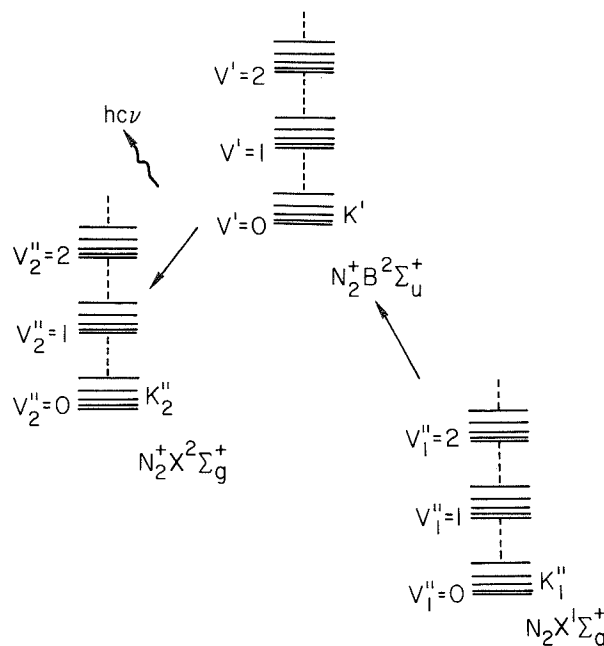
$V' = 2$

$hc\nu$

$V' = 1$

$V' = 0$ $\quad K'$

$V_2'' = 2$

$N_2^+ B\,^2\Sigma_u^+$

$V_2'' = 1$

$V_2'' = 0$ $\quad K_2''$

$N_2^+ X\,^2\Sigma_g^+$

$V_1'' = 2$

$V_1'' = 1$

$V_1'' = 0$ $\quad K_1''$

$N_2 X\,^1\Sigma_g^+$

Figure 1.- Partial energy-level diagram of nitrogen.

The spectral distribution of the $N_2^+(0\text{-}0)$ vibrational band in the first negative system of nitrogen was used in making the rotational-temperature measurements because of the relatively high level of emission intensity in this particular band.

DESCRIPTION OF TECHNIQUE

Figure 2 is a schematic of the instrument in place with the primary experimental apparatus. The instrument is basically a 0.5-meter, f/5.5 dual-channel modified Czerny-Turner spectrometer with a single entrance slit. Fluorescence from the electron beam in the chamber is gathered by a lens and focused onto the variable-width entrance slit, behind which a beam splitter divides the input signal into two parts — one to each channel of the spectrometer. The grating-mirror system in each channel constructs a spectrum at each exit plane; the part of each spectrum detected by the phototubes is determined by adjusting the grating positions and placing fixed-sized exit slits in each exit plane to delimit the width of the spectrum detected.

Before meaningful measurements could be made with the dual-channel system, it was necessary to compensate for the problem of unequal optical efficiencies in each channel. A standard tungsten lamp was placed at the beam position, and the gain of the phototubes was adjusted to give a specific ratio in output signal from the two phototubes. The calibration curve of the standard lamp was integrated over the same two wavelength intervals as defined by the exit slits; the one integrated interval was divided by the other to

PHOTOMULTIPLIER HOUSING

QUARTZ VIEWING PORT

ENTRANCE SLIT ASSEMBLY

ELECTRON BEAM

GATHERING LENS

PRESSURE TEMPERATURE CONTROLLED CHAMBER

PHOTOMULTIPLIER HOUSING

1. Collimating mirror
2. Grating
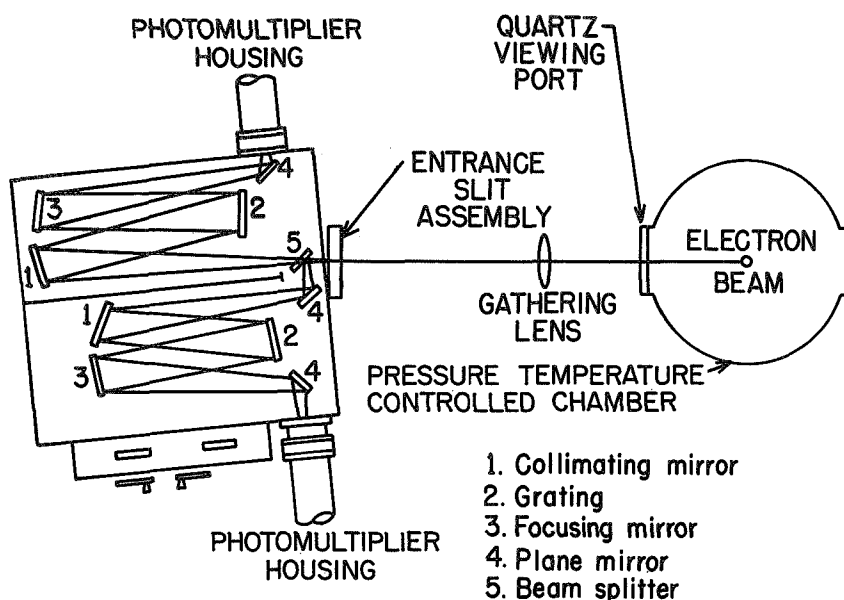3. Focusing mirror
4. Plane mirror
5. Beam splitter

Figure 2.- Diagram of spectrometer and primary experimental apparatus.

give the specified ratio used as a reference. The calibration of the two phototubes was checked periodically for drifting although the drift was found to be quite small. The grating positions in each channel were calibrated by using the 3888.65 Å (1 angstrom = 10^{-10} meter) helium line as a reference.

The relative distribution of rotational energy in the vibrational band between the two channels is a calculable function of the rotational temperature; as the rotational temperature changes, the ratio of spectral energy between the two channels also changes. It is this ratio which is characteristic of the particular temperature.

For the development of the ratio as a function of temperature, attention must be paid to the shape of the observed spectral lines at the instrument exit slit. In the present experiment, approximate exit-plane considerations of the spectrum are discussed in the section entitled "Theoretical Calculations Based on Model Spectrum." It should be noted that the source did not provide a uniform illumination of the entrance slit. Hence, the source geometry plays a complicating role for this particular arrangement, which would not occur in other circumstances. The electron beam produces fluorescence of roughly cylindrical symmetry, which has a diameter of about 1 millimeter or less at the point of observation for nitrogen number densities below 1.5×10^{22} m^{-3}. By use of a 400-μm entrance slit width and a condensor lens magnification of about 0.5, a sufficient part of the beam cross section is observed to result in spatial nonuniformity across the slit. Therefore, the particular source distribution must be accounted in developing model spectrum calculations.

THEORETICAL CALCULATIONS BASED ON MODEL SPECTRUM

In order to calculate the ratio to be expected for any given rotational temperature, it was necessary to construct a model nitrogen spectrum on a computer. Relative line strengths were calculated as a function of rotational temperature on the basis of the work developed by E. P. Muntz (ref. 1). Relative line strengths in the $N_2^+(0-0)$ vibrational transitions are related to the rotational temperature by the equations (ref. 2)

$$I_{K',K'-1} = \frac{K'}{2K'+1}\left\{ K' \exp\left[-B_0 hc K' \frac{(K'-1)}{kT_r}\right] \right.$$

$$\left. + (K'+1)\exp\left[-B_0 hc(K'+1)\frac{(K'+2)}{kT_r}\right]\right\} W_k \qquad \text{(R branch)} \qquad (1)$$

$$I_{K',K'+1} = \frac{K'+1}{K'} I_{K',K'-1} \qquad \text{(P branch)} \qquad (2)$$

except for

$$I_{0,1} = \frac{1}{2}\exp\frac{-B_0 hc2}{kT_r} \qquad (3)$$

where

B_0 rotational constant for the $V_1'' = 0$ level

K' rotational quantum number of the initial state

$$W_k = \begin{cases} 1 & K' \text{ odd} \\ \frac{1}{2} & K' \text{ even} \end{cases}$$

h   Planck's constant

k   Boltzmann's constant

c   speed of light

T_r rotational temperature

When the line strengths had been calculated, it was necessary to approximate the effect of the nonuniformity of the illumination incident on the entrance slit and the effect of the apparatus function on the slit images in the exit plane. For this purpose, various

Voigt profiles were used to obtain systematic changes of the model in the exit plane. These particular profiles were considered useful, although somewhat artificial, on the basis of observations of the actual line and band shapes at the exit plane. A combination of slits with 400-μm entrance and 10-μm exit widths were used with the electron beam source to make the observations.

Initially the second approximation to the exact solution of the Voigt profile given by Whiting (ref. 3), seen in the following equation, was used to describe the spectral distribution of energy in each line at the exit plane:

$$\frac{I_\lambda}{I_{\lambda_{\mathbb{C}}}} = \left(1 - \frac{W_l}{W_v}\right)\exp\left[-2.772\left(\frac{\lambda - \lambda_{\mathbb{C}}}{W_v}\right)^2\right] + \left(\frac{W_l}{W_v}\right)\frac{1}{1 + 4\left(\frac{\lambda - \lambda_{\mathbb{C}}}{W_v}\right)^2}$$

$$+ 0.016\left(1 - \frac{W_l}{W_v}\right)\left(\frac{W_l}{W_v}\right)\left\{\exp\left[-0.4\left(\frac{\lambda - \lambda_{\mathbb{C}}}{W_v}\right)^{2.25}\right] - \frac{10}{10 + \left(\frac{\lambda - \lambda_{\mathbb{C}}}{W_v}\right)^{2.25}}\right\} \qquad (4)$$

where

I_λ	intensity at a wavelength λ
$I_{\lambda_{\mathbb{C}}}$	intensity at the center wavelength
$\lambda_{\mathbb{C}}$	center-line wavelength
W_v	Voigt width at half-height
W_l	Lorentz width at half-height

As can be seen in table 1, the values obtained by use of the first approximation of the exact solution to the Voigt profile (ref. 3) given by

$$\frac{I_\lambda}{I_{\lambda_{\mathbb{C}}}} = \left(1 - \frac{W_l}{W_v}\right)\exp\left[-2.772\left(\frac{\lambda - \lambda_{\mathbb{C}}}{W_v}\right)^2\right] + \left(\frac{W_l}{W_v}\right)\frac{1}{1 + 4\left(\frac{\lambda - \lambda_{\mathbb{C}}}{W_v}\right)^2}$$

are very close to those obtained from the more complex second approximation. Of even more interest is the fact that except for the lowest temperatures, the results from the Voigt profiles are more nearly equal those obtained in the laboratory for a ratio of $W_l/W_v = 0.0$, for which the Voigt profile reduces to a pure Gaussian profile.

Further development of the effect of the choice of the apparatus function on the computed results is not within the scope of this paper, except to mention that the width of the apparatus function used in the computations was determined experimentally for each channel.

Figure 3 shows a comparison of a computer plot of the theoretical model spectrum of the N_2^+(0-0) and N_2^+(1-1) vibrational bands at a rotational temperature of 150° K for two entrance slit widths by using a Gaussian profile for each individual line. The calculations of band intensities followed the procedure of references 1 and 2. It should be pointed out that the N_2^+(1-1) band is present with the 25-μm entrance slit (0.20 Å line width), but on the scale chosen for the spectrum, the band was too small to illustrate. The dashed lines represent the wavelength intervals defined by each exit slit. The theoretical ratio was calculated by integrating the spectral intensity from 3885.2 Å to 3905.5 Å and dividing this result by the integrated intensity between 3905.5 Å and 3910.2 Å — the limits being those defined by the widths of the exit slits. For the 400-μm entrance slit (3.50 Å line width), it was necessary to include part of the N_2^+(1-1) vibrational band, since it overlapped into the lower limit of one of the exit slits.

Figure 4 illustrates a computer plot of the model spectrum at a rotational temperature of 500° K for the same entrance slit widths as in figure 3. The effect of the N_2^+(1-1) band can be seen to be even more significant at the higher rotational temperature, since it
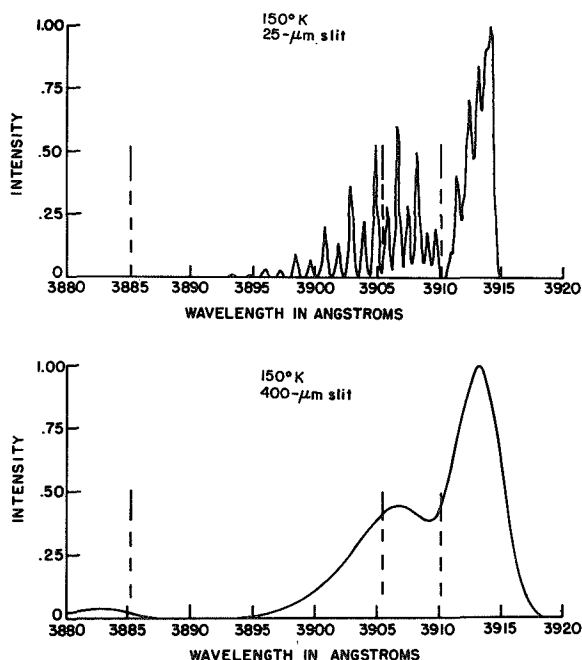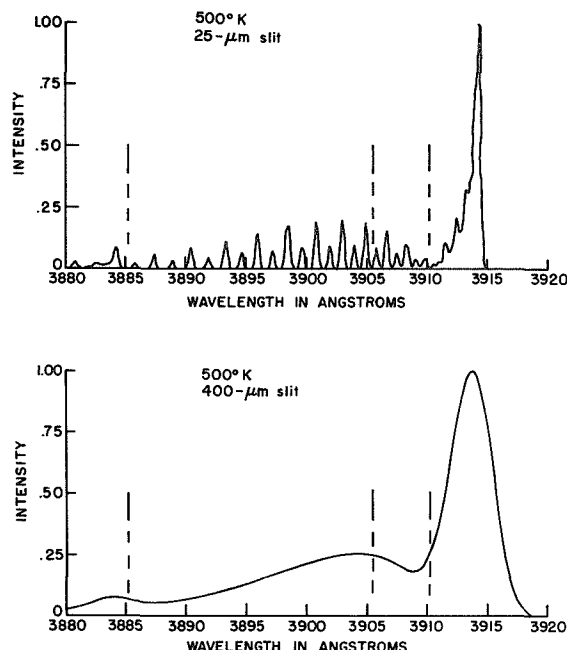

Figure 3.- Plot of theoretical model spectra of N_2^+(0-0) and N_2^+(1-1) vibrational bands at a rotational temperature of 150° K for two entrance slit widths.

Figure 4.- Plot of theoretical model spectra of $N_2^+(0\text{-}0)$ and $N_2^+(1\text{-}1)$ vibrational bands at a rotational temperature of 500° K for two entrance slit widths.

was assumed that the vibrational and rotational modes were in equilibrium for the calculations. If the two were not in equilibrium, it would be necessary to change the relative band intensities accordingly.

Initially it had been intended to use the instrument with a 25-μm entrance slit to give the best resolution at the exit slits; however, it was found that the increase in signal with a 400-μm entrance slit was worth the trade-off in resolution. The effect of two entrance slit widths on the calculations of the ratio as a function of temperature can be seen in figure 5. Because of the particular choice of exit slits, the bow in the upper part of the curves limits the usefulness of the instrument to temperatures below 550° K.

RESULTS AND DISCUSSION

Figure 6 shows the theoretical curve for the 400-μm entrance slit plotted with the data obtained with that slit. The temperatures were determined by scanning the $N_2^+(0\text{-}0)$ vibrational band in the first negative system of nitrogen with a 0.5-meter Ebert spectrometer; from the resolved spectrum, the rotational temperatures could be determined from the relative spectral intensities (ref. 2). The ratios in output levels from the two channels were plotted against the rotational temperatures determined from the scanning spectrometer. The uncertainties for the data points shown without error bars were smaller than
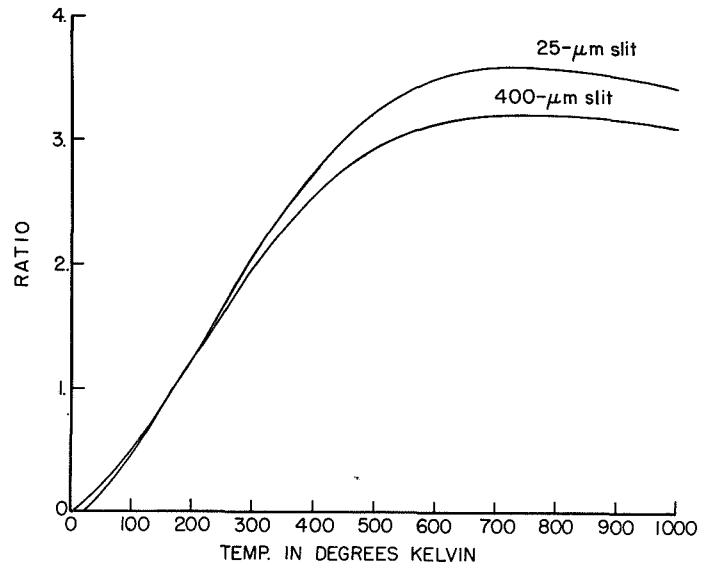
Figure 5.- Comparison of theoretical results for
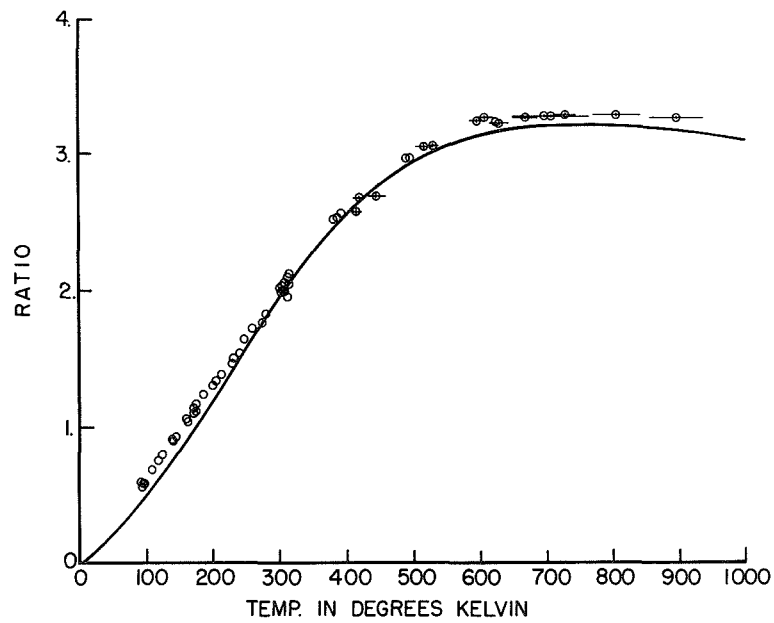25- and 400-μm entrance slits.

Figure 6.- Comparison of experimental data for
400-μm entrance slit with theoretical results
for 400-μm entrance slit.

the circles for those particular measurements. For almost all data points, the ratio could be determined within ±1 percent. For higher temperatures, the rotational energy in the resolved spectra was spread among so many lines that it was difficult to read each line intensity with sufficient accuracy for better measurements. The indicated error bars at the higher temperatures are the 1-sigma deviations in the determination of the rotational temperature by use of the scanning spectrometer.

The uncertainties discussed herein do not include errors which would be introduced if the rotational and vibrational temperatures had not been in equilibrium. Since no measurements described in this report were at other than equilibrium, calculations were made to determine the effect on nonequilibrium. As a worst case, for an entrance slit of 400 μm, rotational temperature of 100° K, and vibrational temperature of 2100° K, the ratio increased by only 3 percent over that when the rotational and vibrational temperatures were both 100° K. This increase in ratio appears to indicate a temperature of about 104° K. It is also possible to choose exit slits of a different width in order to exclude the overlapping into the lower limit when a wide entrance slit is used. Because of the versatility of the instrument, there is no reason that it could not be calibrated for making vibrational-temperature measurements.

The instrument would be especially useful for low temperatures, which might be encountered in the core of the test gas flowing in a hypersonic wind-tunnel facility. The time resolution of the dual-channel spectrometer is a significant improvement over the slower scanning method of temperature determination. Preliminary investigation has shown that it is possible to make a temperature measurement within ±10 to 15 percent for test times of 1 millisecond.

CONCLUDING REMARKS

An instrument for measuring rotational temperatures of low-density $(1.5 \times 10^{22}$ m$^{-3})$ nitrogen gas has been developed. The useful tested range was from about 80° K to 550° K although a different choice of exit slits could easily raise the upper range of temperature measurement.

Although the instrument could be used independently of any theoretical reduction of data, the theoretical calculations presented herein have verified the method used as well as provided information about conditions which could not be obtained in the laboratory. An improvement of the instrument performance at laboratory conditions was realized by using a 400-μm entrance slit width. The system was examined under rather special experimental conditions, particularly with regard to spectrometer illumination. Further

effort is required to fully examine the capability of the instrument, especially with regard to distinguishing the effects of spatial source distribution from the instrument function.

Langley Research Center,
      National Aeronautics and Space Administration,
            Hampton, Va., October 9, 1970.

REFERENCES

1. Muntz, E. P.: Measurement of Rotational Temperature, Vibrational Temperature, and Molecule Concentration, in Non-Radiating Flows of Low Density Nitrogen. Rep. No. 71 (AFOSR TN 60-499), Inst. Aerophys., Univ. of Toronto, Apr. 1961.

2. Hunter, William W., Jr.: Investigation of Temperature Measurements in 300° to 1100° K Low-Density Air Using an Electron Beam Probe. NASA TN D-4500, 1968.

3. Whiting, E. E.: An Empirical Approximation of the Voigt Profile. J. Quant. Spectry. Radiat. Transfer, vol. 8, no. 6, June 1968, pp. 1379-1384.

TABLE I.- RATIOS AS A FUNCTION OF ROTATIONAL TEMPERATURE

Rotational temperature, °K	Experimental ratio	Approximation		Ratios for W_l/W_v of —					
				[a]0.0	0.2	0.4	0.6	0.8	[b]1.0 (c)
100	0.61	{	First	0.51	0.57	0.62	0.66	0.70	0.73
			Second	.51	.56	.59	.63	.66	.69
200	1.30	{	First	1.24	1.26	1.28	1.30	1.31	1.32
			Second	1.24	1.25	1.26	1.27	1.28	1.28
300	1.98	{	First	1.95	1.92	1.89	1.87	1.85	1.83
			Second	1.95	1.91	1.88	1.85	1.82	1.80
400	2.56	{	First	2.54	2.45	2.37	2.31	2.26	2.22
			Second	2.54	2.44	2.36	2.30	2.24	2.20
500	2.97	{	First	2.94	2.80	2.69	2.60	2.53	2.47
			Second	2.94	2.80	2.69	2.59	2.52	2.45
600	3.24	{	First	3.14	2.98	2.86	2.76	2.68	2.61
			Second	3.14	2.98	2.86	2.76	2.67	2.60
700	3.28	{	First	3.21	3.05	2.93	2.83	2.75	2.69
			Second	3.21	3.05	2.93	2.83	2.74	2.67
800	3.29	{	First	3.20	3.06	2.94	2.85	2.78	2.71
			Second	3.20	3.06	2.94	2.85	2.77	2.70

[a]Gaussian value.

[b]Lorentzian value.

[c]The reason the first and second approximations are not equal in the Lorentzian limit is in the definition of center-line intensity.

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